Table D6. Individual hydrocarbon and total petroleum hydrocarbon concentrations (in µg/g wet wt.) for ribbed mussels taken from Con Edison Tower marsh, an unplanted site.[1-3]

Sample ID	Nonane (n-C$_9$)	Decane (n-C$_{10}$)	Undecane (n-C$_{11}$)	Dodecane (n-C$_{12}$)	Tridecane (n-C$_{13}$)	Tetradecane (n-C$_{14}$)	Pentadecane (n-C$_{15}$)	Hexadecane (n-C$_{16}$)	Heptadecane (n-C$_{17}$)	Pristane	Octadecane (n-C$_{18}$)	Phytane	Nonadecane (n-C$_{19}$)	Eicosane (n-C$_{20}$)	Heneicosane (n-C$_{21}$)	Docosane (n-C$_{22}$)	Tricosane (n-C$_{23}$)
First Collection																	
197020421	0.41	nd	nd	nd	nd	nd	nd	0.13	0.20	nd	nd	nd	nd	nd	1.36	nd	nd
197020422	1.21	nd	nd	nd	nd	nd	nd	0.11	0.23	0.15	nd	nd	0.19	nd	1.91	nd	nd
197020423	0.73	nd	nd	nd	nd	nd	nd	nd	0.15	nd	nd	nd	nd	nd	0.88	nd	nd
197020425	0.49	nd	nd	nd	nd	nd	nd	nd	0.08	nd	nd	nd	nd	nd	nd	0.94	nd
297031701	nd	nd	nd	nd	nd	nd	nd	nd	0.26	0.12	nd	0.10	0.57	nd	0.94	nd	2.61
Average[4]	0.59	nd	nd	nd	nd	nd	nd	< MDL	0.18	< MDL	nd	< MDL	0.18	nd	1.06	< MDL	< MDL
Std Dev	0.41	-	-	-	-	-	-	-	0.07	-	-	-	0.22	-	0.64	-	-
Second Collection																	
497051422	0.25	nd	nd	nd	nd	nd	nd	nd	1.07	0.24	nd	0.18	0.92	nd	1.47	nd	nd
497051423	nd	nd	nd	nd	nd	nd	nd	nd	0.88	0.17	nd	0.12	0.14	nd	2.78	nd	2.50
497051424	nd	nd	nd	nd	nd	nd	nd	nd	0.75	nd	nd	0.15	nd	nd	1.33	nd	2.80
497051425	3.01	nd	nd	nd	nd	0.13	0.16	nd	5.65	0.41	0.13	0.75	7.62	0.66	12.6	4.80	10.9
497051426	nd	nd	nd	nd	nd	nd	nd	nd	0.95	nd	nd	0.14	0.15	nd	2.14	nd	nd
Average[4]	0.73	nd	nd	nd	nd	< MDL	< MDL	nd	1.86	0.18	< MDL	0.27	1.78	0.22	4.07	1.23	3.73
Std Dev	1.28	-	-	-	-	-	-	-	2.12	0.15	-	0.27	3.29	0.25	4.81	1.99	4.06
MDL	0.24	0.06	0.12	0.12	0.11	0.11	0.11	0.09	0.08	0.10	0.10	0.10	0.11	0.21	0.38	0.68	2.47

Table D6. Continued.[1-3]

Sample ID	Tetracosane (n-C_{24})	Pentacosane (n-C_{25})	Hexacosane (n-C_{26})	Heptacosane (n-C_{27})	Octacosane (n-C_{28})	Nonacosane (n-C_{29})	Triacontane (n-C_{30})	n-Hentriacontane (n-C_{31})	Dotriacontane (n-C_{32})	Tritriacontane (n-C_{33})	Tetratriacontane (n-C_{34})	Pentatriacontane (n-C_{35})	Hexatriacontane (n-C_{36})	Heptatriacontane (n-C_{37})	Octatriacontane (n-C_{38})	Nonatriacontane (n-C_{39})	Tetracontane (n-C_{40})
First Collection																	
197020421	nd	nd	nd	0.08	nd	nd	nd	64.5	3.13	3.31	0.58	0.60	0.57	0.54	0.42	0.31	0.19
197020422	nd	nd	nd	nd	nd	nd	nd	0.52	0.89	0.65	0.49	0.55	0.51	0.52	0.39	0.29	0.18
197020423	nd	nd	nd	nd	nd	nd	nd	0.23	0.20	0.28	0.32	0.39	0.37	0.36	0.30	0.22	0.14
197020425	nd	nd	nd	nd	nd	nd	nd	0.13	nd	0.18	0.15	0.17	0.16	nd	0.12	0.09	0.06
297031701	nd	nd	nd	nd	nd	nd	nd	nd	nd	0.21	nd	0.12	nd	nd	0.10	0.14	0.16
Average[4]	nd	nd	nd	< MDL	nd	nd	nd	13.1	0.87	0.93	0.32	0.37	0.33	0.32	0.27	0.21	0.15
Std Dev	-	-	-	-	-	-	-	28.8	1.31	1.35	0.22	0.22	0.22	0.22	0.15	0.09	0.05
Second Collection																	
497051422	nd	nd	nd	nd	nd	nd	nd	0.24	0.81	0.34	nd	0.11	0.11	nd	0.15	0.06	nd
497051423	nd	nd	nd	nd	nd	nd	nd	0.13	nd	nd	nd	0.14	0.12	nd	0.13	0.08	nd
497051424	nd	nd	nd	0.35	0.31	4.30	0.62	nd	0.22	nd	nd	nd	nd	nd	nd	nd	nd
497051425	0.44	0.95	0.45	nd	nd	nd	nd	0.28	nd	nd	nd	nd	nd	nd	0.10	0.06	nd
497051426	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	0.12	nd	nd	0.10	0.06	nd
Average[4]	< MDL	0.30	0.13	0.10	< MDL	1.08	< MDL	0.15	0.25	0.11	nd	< MDL	< MDL	nd	0.10	0.06	nd
Std Dev	-	0.36	0.17	0.14	-	1.80	-	0.10	0.32	0.13	-	-	-	-	0.04	0.02	-
MDL	0.29	0.27	0.11	0.08	0.20	0.56	0.48	0.11	0.14	0.11	0.09	0.10	0.10	0.18	0.08	0.06	0.06

Table D6. Continued.[1-3]

Sample ID	Total Petroleum Hydrocarbons[5]	Total Concentrations of Individual Hydrocarbons[6,7,15]	TOTAL: Pristane + Phytane[6,15]	Pristane/n-C_{17}[16]	Phytane/n-C_{18}[16]	Pristane/Phytane[16]	Total: Odd No Carbons[6,8,15]	Total: Even No Carbons[6,9,15]	Carbon Preference Index (CPI)[10,16]	Sum: C_{10}-C_{12}-C_{14}[6,11,15]	Sum: C_{22}-C_{24}-C_{26}-C_{28}[6,12,15]	Weathering Index (WI)[13,16]
First Collection												
197020421	195	79.5	nd	-	-	-	73.2	6.21	11.8	nd	nd	-
197020422	161	11.9	nd	0.64	-	-	7.92	3.76	2.11	nd	nd	-
197020423	83.6	nd	nd	-	-	-	5.15	nd	-	nd	nd	-
197020425	nd	nd	nd	-	-	-	nd	nd	-	nd	nd	-
297031701	63.1	nd	0.21	0.45	-	1.20	5.74	nd	-	nd	nd	-
Average[4]	106	22.5	< MDL	-	-	-	19.1	3.31	5.76 [17]	nd	nd	-
Std Dev	70.0	31.9	-	-	-	-	30.3	1.78	-	-	-	-
Second Collection												
497051422	135	9.20	0.42	0.22	-	1.35	6.41	nd	-	nd	nd	-
497051423	144	9.44	0.29	0.19	-	1.43	7.54	nd	-	nd	nd	-
497051424	235	12.7	0.20	-	-	-	10.3	nd	-	nd	nd	-
497051425	274	50.4	1.16	0.07	5.66	0.55	41.8	7.37	5.68	nd	5.79	-
497051426	115	nd	nd	-	-	-	5.60	nd	-	nd	nd	-
Average[4]	181	17.8	0.45	0.10 [17]	-	0.69 [17]	14.3	3.02	4.75 [17]	nd	1.71	-
Std Dev	69.5	18.3	0.41	-	-	-	15.5	2.46	-	-	2.28	-
MDL	53.6	8.19[14]	0.19[14]				5.09[14]	2.91[14]		0.29[14]	1.29[14]	

Table D6. Continued.

Footnotes:

1   The concentrations of the individual aliphatic hydrocarbons and the total petroleum hydrocarbons were determined using external standard calculations.

2   When an individual aliphatic hydrocarbon was not detected, its concentration was replaced by nd.

3   The concentrations for n-C_8 will be not reported, since it was difficult to identify this peak in samples and to determine MDL for n-C_8.

4   If all concentrations are nd, the average is replaced with nd. When there is at least one number in the data set to be averaged, each nd is replaced with 1/2*MDL, and an average is calculated. If this numeric value is less than the MDL, the average is replaced by < MDL; otherwise, the average is the calculated value. When a numeric value is found for the average, the standard deviation is then determined using the same number set used to calculate the average.

5   Determined from the total peak areas in the chromatogram from n-C_8 to n-C_{40} minus any contributions from the internal standard areas.

6   These formulae use 1/2MDL values for each analyte not detected.

7   Sum of the concentrations of the individual aliphatic hydrocarbons n-C_9 through n-C_{40} plus the concentrations of pristane and phytane.

8   The total of the concentrations of the aliphatic hydrocarbons with an odd number of carbon atoms.

9   The total of the concentrations of the aliphatic hydrocarbons with an even number of carbon atoms. The contribution of n-C_8 is not included in the total.

10   Carbon Preference Index (CPI) is defined as the ratio of the total of the concentrations of the aliphatic hydrocarbons with an odd number of carbons to the total concentration of the alphatic hydrocarbons with an even carbon number.

11   The total of the concentrations of n-C_{10}, n-C_{12}, and n-C_{14}.

12   The total of the concentrations of n-C_{22}, n-C_{24}, n-C_{26}, and n-C_{28}.

13   Weathering Index (WI) is defined as the ratio of the total concentration of n-C_{10}, n-C_{12}, and n-C_{14} to the total concentration of n-C_{22}, n-C_{24}, n-C_{26}, and n-C_{28}.

14   These MDL values are calculated with the same summation formulae as the samples using the individual hydrocarbon MDL values.

15   The summation totals for the samples are compared with calculated MDL values obtained using the same summation formulae as the samples. When these sample totals were less than the total MDL, its value was replaced by nd. The averages and standard deviations for the totals were treated in the same way as the individual hydrocarbons; see footnote 4.

16   Numerical values of the CPI, WI, and the ratios: pristane/n-C_{17}, phytane/n-C_{18}, and pristane/phytane, will be calculated only when the defined quantity for each index or ratio has a numeric value.

17   These results are not true averages, instead they are the ratios of the averages of the defined quantities, if these averages exist.